NATIONAL UNIVERSITY OF SINGAPORE

PC5202 ADVANCED STATISTICAL MECHANICS

(Semester II: AY 2014-15)

Time Allowed: 2 Hours

INSTRUCTIONS TO STUDENTS

1. Please write your student number only. Do not write your name.
2. This assessment paper contains 5 questions and comprises 3 printed pages.
3. Students are required to answer ALL the questions.
4. Students should write the answers for each question on a new page.
5. This is a CLOSED BOOK examination.
6. Each question carries 20 marks.

1. For each of the following multiple choice questions, indicate one only from among A to E as the best answer.

   i. In a classical micro-canonical ensemble the phase space distribution function

      A. ρ is a constant on a hypersurface $H(p,q) = E$.
      B. ρ is a constant in the region $H(p,q) < E$.
      C. ρ is proportional to energy E.
      D. ρ is proportional to $\exp(-\beta H)$.
      E. ρ is proportional to $\delta(H(p,q) - E)$.

   ii. The Jarzynski relation connecting work W with Helmholtz free energy F is

      A. $\langle e^{-\beta W} \rangle > e^{-\beta \Delta F}$.
      B. $\langle e^{-\beta W} \rangle < e^{-\beta \Delta F}$.
      C. $\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$.
      D. $\langle e^{-\beta W} \rangle = e^{-\beta F}$.
      E. $\langle e^{\beta W} \rangle = e^{\beta \Delta F}$.

   iii. With the scaling hypothesis, $f(b^Y t, b^X h) = b^D f(t,h)$, for the singular part of the free energy per degree of freedom near critical point, which one of the following statements is not true or not implied?

      A. D is the dimension of the system.
      B. t is $T - T_C$.
      C. Widom's scaling law, $\beta(\delta - 1) = \gamma$.
      D. Fisher's scaling law, $\gamma = (2 - \eta)\nu$.
      E. Rushbrooke's scaling law, $\alpha + 2\beta + \gamma = 2$.

   iv. In a quantum ideal Bose gas, the critical Bose-Einstein condensation temperature T_0 at which the occupation number of the ground state acquired an average value $\langle n_0 \rangle$ of order N (the number of particles of the system) can be estimated approximately by

      A. $k_B T_0 \approx \hbar\omega$.
      B. $k_B T_0 \approx \hbar^2 / \left(2m(\frac{V}{N})^{\frac{2}{3}}\right)$.
      C. $k_B T_0 \approx \hbar^2/(2mV^{\frac{2}{3}})$.
      D. $k_B T_0 \approx \langle mv^2 \rangle$.
      E. $k_B T_0 \approx 8a/(27b)$.

   v. Einstein equation is

      A. $E = mc^2$.
      B. $\langle x^2 \rangle = 2Dt$.
      C. $D = k_B T/(6\pi\eta a)$.
      D. $D = \mu k_B T$.
      E. All of the above.

i)E, ii) C, iii) D, iv) B, v) E.

2. The eigen-energies of a single quantum particle in a one-dimensional box is $E_n = \frac{\pi^2\hbar^2 n^2}{2mL^2}$, where $n = 1, 2, 3, \ldots$, and m is mass, L is the length of the interval where the particle is confined. Working in canonical ensemble:
   i. Determine the force that the particle exerts to the wall of the box, in the high-temperature limit, i.e., $\beta = 1/(k_B T)$ is small.
   ii. Determine the same force, but in the opposite limit, i.e., temperature T is small. The answer should be accurate to the first order of a suitable small low-temperature expansion parameter.

   Define $\alpha = \frac{\pi^2\hbar^2}{2m}$*, then* $E_n = \alpha n^2/L^2$*, the partition function is* $Z = \sum_{n=1}^{\infty} e^{-\beta\alpha n^2/L^2} = x + x^4 + x^9 + \cdots$*, where* $x = e^{-\alpha\beta/L^2}$*. For low temperatures,* $\beta = 1/(k_B T)$ *is large, and* x *is small, we just keep the first two terms in the Taylor expansion of* x *as a good approximation. For higher temperature, the summand varies slowly with* n *we approximate the sum by integral,* $Z \approx \int_0^{\infty} e^{-\frac{\alpha\beta n^2}{L^2}}\, dn = L\sqrt{2\pi m\, k_B T}\,/h$*, (exactly the same result as for in classical particle, i.e.,* $\iint \frac{dxdp}{h} e^{-\frac{\beta p^2}{2m}}$*) and the free energy is* $F = -k_B T \ln Z$*. Using force* $f = -\frac{\partial F}{\partial L}$*, we obtain, for i) high temperature* $f = k_B T/L$ *(ideal gas law), ii) for low temperature* $f = \frac{2\alpha}{L^3}(1 + 3x^3 + \cdots)$.

3. For exact results in two-dimensional Ising models, duality plays an important role.
   i. Explain the meaning of duality in a topological sense and demonstrate that square lattice is self-dual.
   ii. State the duality relation, which relates high-temperature expansion with low-temperature expansion.
   iii. Give the duality argument that the critical temperature of the two-dimensional Ising model on a square lattice with nearest neighbor interaction is determined by $\tanh K_c = \exp(-2K_c)$, where $K_c = J/(k_B T_c)$.

   Exactly the same as in my notes, or at the elearning-week recordings.

4. Consider the Langevin equation in the case where the acceleration term mdv/dt is negligible, $-k\frac{dx}{dt} + R(t) = 0$, with a standard white noise for the random force, i.e., $\langle R(t)\rangle = 0$, $\langle R(t)R(t')\rangle = C\delta(t - t')$.

i. Solve the stochastic differential equation assuming the initial condition $x(0) = 0$; determine the mean-square displacement $\langle x(t)^2 \rangle$ as a function of time t.

ii. Derive the Fokker-Planck equation for the probability density $\langle P(x,t) \rangle$ for the random variable x.

i) *Integrate, we get* $x(t) = \frac{1}{k} \int_0^t R(t')dt'$. *Perform a two-dimensional integral over a square of* $[0,t]^2$ *and the use the delta function correlation, we obtain,* $\langle x(t)^2 \rangle = 1/k^2 \int_0^t dt_1 \int_0^t dt_2 \langle R(t_1)R(t_2) \rangle = Ct/k^2$.

ii) *Probability conservation means* $\frac{\partial P}{\partial t} + \frac{\partial}{\partial x}(\dot{x}P) = 0$. *Using the expression for the rate of* x, *and moving the second term to the right and solving the equation formally, then taken average over noise, or alternatively, using analogy to the standard Fokker-Planck equation, we obtain (skipping steps),* $\frac{\partial \langle P(x,t) \rangle}{\partial t} = \frac{C}{2k^2} \frac{\partial^2}{\partial x^2} \langle P(x,t) \rangle$ *, which is a diffusion equation.*

5. Consider a simplified Boltzmann equation of the form $\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_{\boldsymbol{r}} f = -\frac{f - f_{\mathrm{eq}}}{\tau}$, where f_{eq} is local equilibrium distribution having the property $\langle \ln f_{\mathrm{eq}} \rangle_f = \langle \ln f_{\mathrm{eq}} \rangle_{f_{\mathrm{eq}}}$. m is mass of the particle, $\tau > 0$ is relaxation time constant, and the distribution function $f = f(\boldsymbol{r}, \boldsymbol{p}, t)$ is a function of (three-dimensional) position $\boldsymbol{r}$, momentum $\boldsymbol{p}$, and time t. The Boltzmann H-function is defined as $H = \iint d\boldsymbol{r} d\boldsymbol{p} \, f \ln f$. Prove the H-theorem: $\frac{dH}{dt} \leq 0$.

The key steps are: $\frac{dH}{dt} = \int d\boldsymbol{r} \int d\boldsymbol{p} \frac{\partial f}{\partial t}(1 + \ln f)$. *This is because,* t, $\boldsymbol{r}$, $\boldsymbol{p}$ *are independent variables. Use Boltzmann equation* $\frac{\partial f}{\partial t} = -\frac{\mathbf{p}}{m} \cdot \nabla_{\boldsymbol{r}} f - \frac{f - f_{\mathrm{eq}}}{\tau}$, *the first momentum term can be dropped, because, it can be written as* $\int d\boldsymbol{r} \ \nabla_{\boldsymbol{r}}(f \ln f)$ *and can be changed to a surface integral using Gauss theorem. The 1 can also be dropped because particle number conservation,* $\int d\boldsymbol{r} \int d\boldsymbol{p} \, f = N$. *We are left with* $\frac{dH}{dt} = -\frac{1}{\tau} \int d\boldsymbol{r} \int d\boldsymbol{p} \left(f - f_{\mathrm{eq}}\right) \ln f$. *To proceed further, we use the given local equilibrium condition, which means* $\int d\boldsymbol{r} \int d\boldsymbol{p} \left(f - f_{\mathrm{eq}}\right) \ln \boldsymbol{f_{eq}} = 0$. *Dividing by* τ *, adding into* dH/dt, *we get* $\frac{dH}{dt} = -\frac{1}{\tau} \int d\boldsymbol{r} \int d\boldsymbol{p} \left(f - f_{\mathrm{eq}}\right) \ln \frac{f}{f_{\mathrm{eq}}} \leq 0$. *This problem is an example in the book of R. Zwanzig, page 93-96.*

\- The end - [JSW]